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Sandia National Laboratories

Atomistic Study of Phonon Generation and Evolution by Laser Excitation

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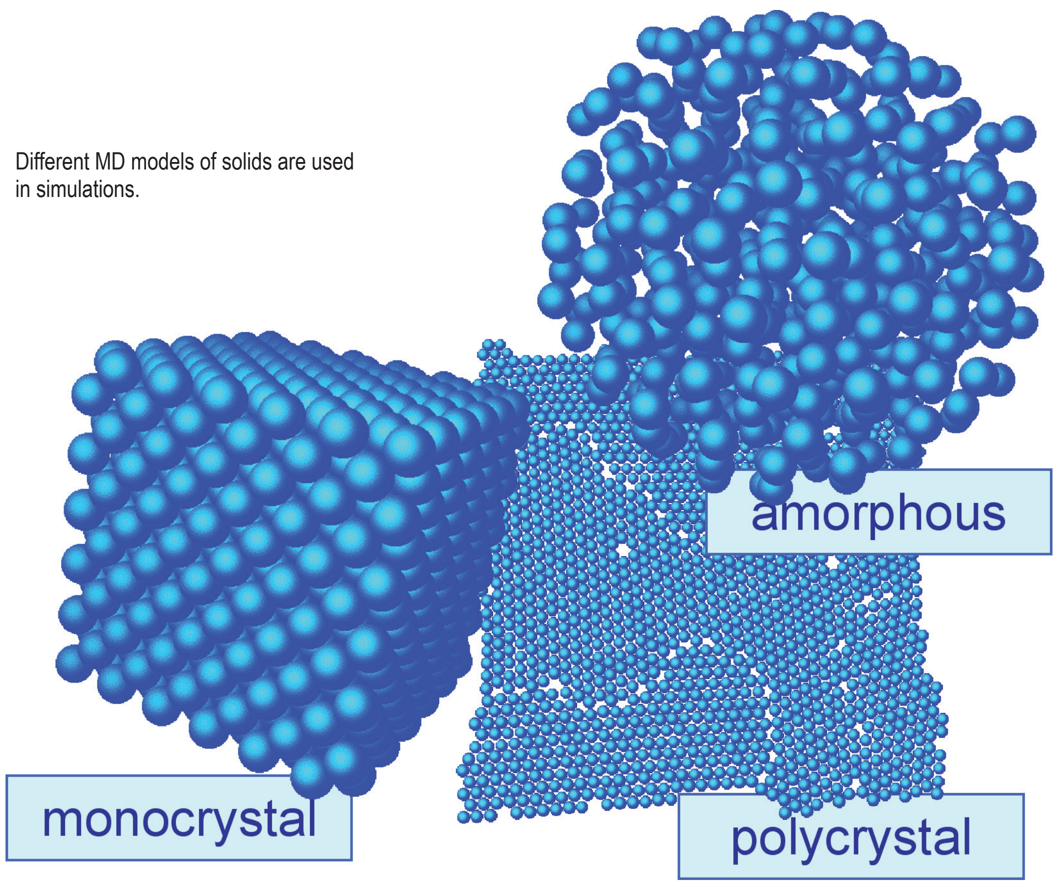
Project Description

An atomistic study of thermal transport by a concentrated energy source will be conducted, including molecular dynamics (MD) simulations. Experiments measuring the transport of heat introduced by laser excitation provide data for guiding and validating numerical results.

Four tasks will be performed at the discretion of the Sandia principal investigator:

- Construct structural-rheological model of a two-component solid appropriate for description of its atomic-corpuscular nature; derive boundary-value problem for a medium with a complex structure; construct nonlinear model for phonon build-up in silicon monocrystal subjected to various conditions; simulation of heat propagation in monocrystal solid.
- Derive dynamical equations and constitutive laws for 3-D solid; model transfer of energy to higher vibratory modes, construct coupled nonlinear equations for low-frequency and high–frequency acoustic field and thermal field interacting with excitons; propagation of heat in polycrystal solid.
- Model ballistic phonon transport.
- Model the characteristics that influence material structure on phonon transport.



Different MD models of solids are used in simulations.

Technical Purpose and Benefits

The use of atomistic simulation brings high fidelity physics into materials modeling. At atomic length and time scales, classical continuum approaches for describing the transport of energy and for differentiating heat from elastic waves become questionable. In atomistics, it is expected that energy transport will be affected by the individual and group behavior of phonons. This project proposes an atomistic study of thermal transport from a concentrated energy source. The goal is to characterize the transport of energy in an atomic lattice including the effects of phonon dispersion, interaction, and decay.

The project will aid in characterizing the distribution and evolution of phonon spectra, density states, decay, and dispersion for dynamic atomistic simulations of the thermomechanical deformation of solids. It will examine the effect of quasi-diffusion on heat transport in dynamic atomistic simulations and investigate the validity of classical continuum approaches for describing thermal conductivity and energy transport in solids. The results are essential to the development of fracture and failure prediction capabilities by providing physical understanding of the energy dissipation and transport processes, for example, at the crack tip.

Signing contract in St. Petersburg—From left to right: Dr. Tony Chen, Ms. Patty Jojola, Professor Belyaev, and Professor Dimitry Indeitsev.

Collaboration between Sandia National Laboratories (SNL), Livermore, CA, USA, and IPME (Research Institute of Mechanical Engineering Problems), St. Petersburg, Russia

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